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A concise redefinition of the solid spherical harmonics and its use in fast multipole methods

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Abstract

Several *fast* algorithms for the approximation of particle-particle interactions by means of multipole expansions in spherical harmonics have appeared recently. In this letter we present a redefinition of the solid spherical harmonics that is real and gives simple expressions for the evaluation of the functions and their derivatives. Application to the *recursive bisection* method [J. M. Pérez-Jordá and W. Yang, Chem. Phys. Lett. **247**, 484 (1995)] greatly improves its performance.

1 Introduction

In a system with N particles, the exact calculation of particle-particle interactions has a cost proportional to N^2. Fortunately, there are faster approximate algorithms with a better scaling with N, such as the *Fast Multipole Method*[1], which is $O(N)$, or the *Tree Codes*[2, 3] and the *Recursive Bisection Method*[4], which are $O(N \log N)$. All three methods use multipole expansions in spherical harmonics in their approximations of particle-particle interactions.

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In this letter, an equivalent formulation for the approximation of particle-particle interactions by means of multipole expansions is presented, based upon a concise redefinition of the solid spherical harmonics. Its main advantage is the compact expressions obtained for the derivatives, from which the forces can be computed very efficiently.

2 Definition

The potential at $\mathbf{r}_1$ due to a unit charge at $\mathbf{r}_2$ can be expanded[5] as

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}=\sum_{l=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}P_l(\cos\gamma), \tag{1}$$

where $\mathbf{r}_<$ ($\mathbf{r}_>$) is the smaller (larger) of $\mathbf{r}_1$ and $\mathbf{r}_2$, and γ is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$. Combining this with the addition theorem[5] for $P_l(\cos\gamma)$ we get the following real multipole expansion,

$$\begin{aligned}\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} &= \sum_{l=0}^{\infty}\left[\frac{P_l^0(\cos\theta_>)}{r_>^{l+1}}\right]\left[r_<^l P_l^0(\cos\theta_<)\right]+2\sum_{l=1}^{\infty}\sum_{m=1}^{l}\Bigg\{ \\ &\left[(l-m)!\frac{P_l^m(\cos\theta_>)\cos(m\phi_>)}{r_>^{l+1}}\right]\left[\frac{r_<^l P_l^m(\cos\theta_<)\cos(m\phi_<)}{(l+m)!}\right]+ \\ &\left[(l-m)!\frac{P_l^m(\cos\theta_>)\sin(m\phi_>)}{r_>^{l+1}}\right]\left[\frac{r_<^l P_l^m(\cos\theta_<)\sin(m\phi_<)}{(l+m)!}\right]\Bigg\},\end{aligned} \tag{2}$$

where P_l^m are associated Legendre functions[6].

The previous expansion suggest the following definitions for two kind of functions $\mathcal{M}_{l,m}^{\pm}$ and $\mathcal{N}_{l,m}^{\pm}$. Given a point in space $\mathbf{r}$ with spherical polar coordinates r, θ and ϕ, we define the function $\mathcal{M}_{l,m}^{\pm}$ as

$$\mathcal{M}_{l,m}^{+}(\mathbf{r}) = \begin{cases}(l-|m|)!\dfrac{P_l^{|m|}(\cos\theta)\cos|m|\phi}{r^{l+1}} & \text{if } m\geq 0\\ -\mathcal{M}_{l,|m|}^{+}(\mathbf{r}) & \text{if } m<0\end{cases} \tag{3}$$

$$\mathcal{M}_{l,m}^{-}(\mathbf{r}) = (l-|m|)!\frac{P_l^{|m|}(\cos\theta)\sin|m|\phi}{r^{l+1}}, \tag{4}$$

and $\mathcal{N}^{\pm}_{l,m}$ as

$$\mathcal{N}^{+}_{l,m}(\mathbf{r}) = \begin{cases} \dfrac{r^l}{(l+|m|)!} P_l^{|m|}(\cos\theta)\cos|m|\phi & \text{if } m \geq 0 \\ -\mathcal{N}^{+}_{l,|m|}(\mathbf{r}) & \text{if } m < 0 \end{cases} \quad (5)$$

$$\mathcal{N}^{-}_{l,m}(\mathbf{r}) = \frac{r^l}{(l+|m|)!} P_l^{|m|}(\cos\theta)\sin|m|\phi. \quad (6)$$

This definition is somewhat related to the one proposed by White and Head-Gordon[7], although ours is real and the prefactors $(l-|m|)!$ and $(l+|m|)!$ are incorporated in opposite ways.

We will see that a very compact formulation of the particle-particle interaction problem arises from the use of functions $\mathcal{M}^{\pm}_{l,m}$ and $\mathcal{N}^{\pm}_{l,m}$. To begin with, expansion (2) is simplified to

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} = \sum_{l=0}^{\infty} \mathcal{M}^{+}_{l,0}(\mathbf{r}_>)\mathcal{N}^{+}_{l,0}(\mathbf{r}_<) + 2\sum_{l=1}^{\infty}\sum_{m=1}^{l}\left[\mathcal{M}^{+}_{l,m}(\mathbf{r}_>)\mathcal{N}^{+}_{l,m}(\mathbf{r}_<) + \mathcal{M}^{-}_{l,m}(\mathbf{r}_>)\mathcal{N}^{-}_{l,m}(\mathbf{r}_<)\right]. \quad (7)$$

The relationship between $\mathcal{M}^{\pm}_{l,m}$ and $\mathcal{N}^{\pm}_{l,m}$ and the customary solid spherical harmonics is given by:

$$\mathcal{M}^{\pm}_{l,|m|} = i^{(1\mp1)/2} a_{l,m} \frac{Y_l^{-|m|}(\theta,\phi) \pm (-1)^m Y_l^{|m|}(\theta,\phi)}{r^{l+1}} \quad (8)$$

$$\mathcal{N}^{\pm}_{l,|m|} = i^{(1\mp1)/2} \frac{\pi}{a_{l,m}(2l+1)} r^l \left[Y_l^{-|m|}(\theta,\phi) \pm (-1)^m Y_l^{|m|}(\theta,\phi)\right], \quad (9)$$

where

$$a_{l,m} = \sqrt{\frac{\pi(l+|m|)!(l-|m|)!}{2l+1}}. \quad (10)$$

Conversely, we have

$$\frac{Y_l^{|m|}(\theta,\phi)}{r^{l+1}} = (-1)^m \frac{1}{2a_{l,m}}\left[\mathcal{M}^{+}_{l,|m|}(\mathbf{r}) + i\mathcal{M}^{-}_{l,|m|}(\mathbf{r})\right] \quad (11)$$

$$\frac{Y_l^{-|m|}(\theta,\phi)}{r^{l+1}} = \frac{1}{2a_{l,m}}\left[\mathcal{M}^+_{l,|m|}(\mathbf{r}) - i\mathcal{M}^-_{l,|m|}(\mathbf{r})\right] \quad (12)$$

$$r^l Y_l^{|m|}(\theta,\phi) = (-1)^m \frac{a_{l,m}(2l+1)}{2\pi}\left[\mathcal{N}^+_{l,|m|}(\mathbf{r}) + i\mathcal{N}^-_{l,|m|}(\mathbf{r})\right] \quad (13)$$

$$r^l Y_l^{-|m|}(\theta,\phi) = \frac{a_{l,m}(2l+1)}{2\pi}\left[\mathcal{N}^+_{l,|m|}(\mathbf{r}) - i\mathcal{N}^-_{l,|m|}(\mathbf{r})\right]. \quad (14)$$

3 Recurrence relations

The spherical harmonics can be efficiently computed from some well known recurrence relations for the associated Legendre functions[6],

$$P_0^0(\cos\theta) = 1 \quad (15)$$

$$P_{m+1}^{m+1}(\cos\theta) = -(2m+1)\sin\theta P_m^m(\cos\theta) \quad (16)$$

$$P_l^m(\cos\theta) = \frac{(2l-1)\cos\theta P_{l-1}^m(\cos\theta) - (l+m-1)P_{l-2}^m(\cos\theta)}{l-m}. \quad (17)$$

These relations can be easily generalized for $\mathcal{M}^\pm_{l,m}$ and $\mathcal{N}^\pm_{l,m}$. Let x, y, and z be the cartesian coordinates of a point with spherical polar coordinates r, θ, and ϕ. Then, for $\mathcal{M}^\pm_{l,m}$,

$$\mathcal{M}^+_{0,0} = \frac{1}{r} \quad (18)$$

$$\mathcal{M}^-_{0,0} = 0 \quad (19)$$

$$\mathcal{M}^+_{m,m} = -\frac{2m-1}{r^2}\left[x\mathcal{M}^+_{m-1,m-1} - y\mathcal{M}^-_{m-1,m-1}\right] \quad (20)$$

$$\mathcal{M}^-_{m,m} = -\frac{2m-1}{r^2}\left[y\mathcal{M}^+_{m-1,m-1} + x\mathcal{M}^-_{m-1,m-1}\right] \quad (21)$$

$$\mathcal{M}^\pm_{l,m} = \frac{1}{r^2}\left[(2l-1)z\mathcal{M}^\pm_{l-1,m} - (l-1+m)(l-1-m)\mathcal{M}^\pm_{l-2,m}\right]. \quad (22)$$

For $\mathcal{N}^\pm_{l,m}$,

$$\mathcal{N}^+_{0,0} = 1 \quad (23)$$

$$\mathcal{N}^-_{0,0} = 0 \quad (24)$$

$$\mathcal{N}^+_{m,m} = -\frac{1}{2m}\left[x\mathcal{N}^+_{m-1,m-1} - y\mathcal{N}^-_{m-1,m-1}\right] \quad (25)$$

$$\mathcal{N}^-_{m,m} = -\frac{1}{2m}\left[y\mathcal{N}^+_{m-1,m-1} + x\mathcal{N}^-_{m-1,m-1}\right] \quad (26)$$

$$\mathcal{N}^\pm_{l,m} = \frac{1}{(l+m)(l-m)}\left[(2l-1)z\mathcal{N}^\pm_{l-1,m} - r^2\mathcal{N}^\pm_{l-2,m}\right]. \quad (27)$$

Originally, the particles coordinates are given in cartesian coordinates, and we would have to compute the respective spherical polar coordinates. However, if we use the previous recurrence relations,

- there is no need of computing the angles θ and ϕ by inverse trigonometric functions,
- except in $\mathcal{M}^+_{0,0}$, the radius r always appears as r^2. That means that the expensive square root in $r \equiv \sqrt{x^2+y^2+z^2}$ is not required for $\mathcal{N}^\pm_{l,m}$ functions, and is only necessary for $\mathcal{M}^+_{0,0}$.

4 Multipole expansions

Let us suppose that we have two sets of particles $\mathcal{A}$ and $\overline{\mathcal{A}}$. There are N_A particles in $\mathcal{A}$ with charges q_i and positions $\mathbf{r}_i$, and $N_{\overline{A}}$ particles in $\overline{\mathcal{A}}$ with charges $\overline{q}_j$ and positions $\overline{\mathbf{r}}_j$ (it is assumed that the sets are "well-separated"[8]). We will refer to the Coulomb potential energy resulting from the interaction between $\mathcal{A}$ and $\overline{\mathcal{A}}$ as $I[\mathcal{A},\overline{\mathcal{A}}]$,

$$I[\mathcal{A},\overline{\mathcal{A}}] = \sum_{i=1}^{N_A}\sum_{j=1}^{N_{\overline{A}}}\frac{q_i\overline{q}_j}{|\mathbf{r}_i - \overline{\mathbf{r}}_j|}. \quad (28)$$

The interaction between $\mathcal{A}$ and $\overline{\mathcal{A}}$ can be approximated by means of a *multipole expansion*:

$$I[\mathcal{A},\overline{\mathcal{A}}] \approx I^L[\mathcal{A},\overline{\mathcal{A}}] = \sum_{j}^{N_{\overline{A}}}\overline{q}_j\Phi^L_A(\overline{\mathbf{r}}_j), \quad (29)$$

where Φ^L_A is the L-order multipole expansion of the potential created by the set of particles $\mathcal{A}$ (see Eq. (7)),

$$\Phi^L_A(\overline{\mathbf{r}}) = \sum_{l=0}^{L} Q^+_{l,0}\mathcal{M}^+_{l,0}(\overline{\mathbf{r}} - \mathbf{R}_A) + 2\sum_{l=1}^{L}\sum_{m=1}^{l}\left[Q^+_{l,m}\mathcal{M}^+_{l,m}(\overline{\mathbf{r}} - \mathbf{R}_A) + Q^-_{l,m}\mathcal{M}^-_{l,m}(\overline{\mathbf{r}} - \mathbf{R}_A)\right]. \quad (30)$$

The coefficients $Q^{\pm}_{l,m}$ are computed from the particles in $\mathcal{A}$,

$$Q^{\pm}_{l,m} = \sum_{i}^{N_A} q_i \mathcal{N}^{\pm}_{l,m}(\mathbf{r}_i - \mathbf{R}_A). \tag{31}$$

The point $\mathbf{R}_A$ is the center of the multipole expansion.

5 Derivatives

The usefulness of $\mathcal{M}^{\pm}_{l,m}$ and $\mathcal{N}^{\pm}_{l,m}$ is given by the simplicity of their derivatives with respect to cartesian coordinates,

$$\frac{\partial}{\partial x}\mathcal{M}^{\pm}_{l,|m|} = \frac{1}{2}(\mathcal{M}^{\pm}_{l+1,|m|+1} - \mathcal{M}^{\pm}_{l+1,|m|-1}) \tag{32}$$

$$\frac{\partial}{\partial y}\mathcal{M}^{\pm}_{l,|m|} = \frac{\pm 1}{2}(\mathcal{M}^{\mp}_{l+1,|m|+1} + \mathcal{M}^{\mp}_{l+1,|m|-1}) \tag{33}$$

$$\frac{\partial}{\partial z}\mathcal{M}^{\pm}_{l,|m|} = -\mathcal{M}^{\pm}_{l+1,|m|} \tag{34}$$

$$\frac{\partial}{\partial x}\mathcal{N}^{\pm}_{l,|m|} = \frac{1}{2}(\mathcal{N}^{\pm}_{l-1,|m|+1} - \mathcal{N}^{\pm}_{l-1,|m|-1}) \tag{35}$$

$$\frac{\partial}{\partial y}\mathcal{N}^{\pm}_{l,|m|} = \frac{\pm 1}{2}(\mathcal{N}^{\mp}_{l-1,|m|+1} + \mathcal{N}^{\mp}_{l-1,|m|-1}) \tag{36}$$

$$\frac{\partial}{\partial z}\mathcal{N}^{\pm}_{l,|m|} = \mathcal{N}^{\pm}_{l-1,|m|}. \tag{37}$$

These expressions have been obtained from the analogous ones for solid spherical harmonics[9, 10, 4].

The force exerted on particle j in $\overline{\mathcal{A}}$ from all the particles in $\mathcal{A}$ is given by

$$-\frac{\partial}{\partial \overline{x}_j} I[\mathcal{A}, \overline{\mathcal{A}}] \approx -\frac{\partial}{\partial \overline{x}_j} I^L[\mathcal{A}, \overline{\mathcal{A}}] \tag{38}$$

$$-\frac{\partial}{\partial \overline{y}_j} I[\mathcal{A}, \overline{\mathcal{A}}] \approx -\frac{\partial}{\partial \overline{y}_j} I^L[\mathcal{A}, \overline{\mathcal{A}}] \tag{39}$$

$$-\frac{\partial}{\partial \overline{z}_j} I[\mathcal{A}, \overline{\mathcal{A}}] \approx -\frac{\partial}{\partial \overline{z}_j} I^L[\mathcal{A}, \overline{\mathcal{A}}], \tag{40}$$

and, from Eqs. (32)–(37), it is easy to see that the evaluation of the forces involves multipole expansions of order $L+1$ instead of L. For example, for the force z component

$$-\frac{\partial}{\partial \overline{z}_j} I^L[\mathcal{A}, \overline{\mathcal{A}}] = \sum_j^{N_{\overline{A}}} \overline{q}_j \Phi_A^{z,L+1}(\overline{\mathbf{r}}_j), \tag{41}$$

where $\Phi_A^{z,L+1}$ is a $(L+1)$-order multipole expansion with coefficients $\{Q_{l,m}^{z,\pm}\}$

$$Q_{m,m}^{z,\pm} = 0 \tag{42}$$

$$Q_{l+1,m}^{z,\pm} = Q_{l,m}^{\pm}. \tag{43}$$

This set of coefficients can be obtained from $\{Q_{l,m}^{\pm}\}$ by using Eq. (34).

All this suggest the following strategy to compute the potential and forces at the particles in $\overline{\mathcal{A}}$ due to all the particles in $\mathcal{A}$.

Step 1. The coefficients $\{Q_{l,m}^{\pm}\}$ of the multipole expansion Φ_A^L are computed by using the recurrence relations (23)–(27).

Step 2. The coefficients $\{Q_{l,m}^{x,\pm}\}$, $\{Q_{l,m}^{y,\pm}\}$ and $\{Q_{l,m}^{z,\pm}\}$ of the force components multipole expansions $\Phi_A^{x,L+1}$, $\Phi_A^{y,L+1}$ and $\Phi_A^{z,L+1}$ are obtained via (42)–(43) and its analogous for x and y. Note that this step is very fast because it is *not* dependent on the number of particles.

Step 3. The four multipole expansions Φ_A^L, $\Phi_A^{x,L+1}$, $\Phi_A^{y,L+1}$ and $\Phi_A^{z,L+1}$ are evaluated at every particle in $\overline{\mathcal{A}}$ by using the recurrence relations (18)–(22). Note that the $\mathcal{M}_{l,m}^{\pm}$ functions, once computed, can be used by all the multipole expansions. This means that the four multipole expansions are evaluated with a cost considerably smaller than the cost of computing four independent expansions.

6 Application to Fast Multipole Methods

A noticeable fraction of the execution time of a fast algorithm for particle-particle interactions[1, 2, 3, 4] is spent approximating the interactions via multipole expansions. The ideas described here will help the writing of an efficient program for evaluating them. Thus, it is expected that the new scheme will improve significantly the performance of these fast algorithms.

We apply the present algorithm to the Recursive Bisection Method[4]. Our results are shown in table 1 and figure 1. The label "Original" refers to results computed with the program described in Ref. [4]. The label "Present" refers to results computed with the same program, but now modified to implement the ideas explained above. The definition of a "small" set has been slightly changed in the present version. A set of particles was said[4] to be small if it had less than N_0 particles, where

$$N_0 = K(L+2)^2. \tag{44}$$

In the present implementation, the constant K has been set to a new value of 0.40 (that means that a larger fraction of interactions are now evaluated via multipoles). "Direct $O(N^2)$" stands for the exact results computed by direct summation.

In table 1 we see that the error (defined as in Ref. [4]) of both implementations is essentially the same. On the other hand, however, the execution time of the present version (figure 1) has been substantially reduced, up to a 40% for large number of particles.

7 Conclusions

A concise redefinition of the solid spherical harmonics that allows the writing of very efficient code for approximating particle-particle interactions via multipole expansions has been described. It speeds up the Recursive Bisection Method[4] up to 40%.

The program is available from the authors by request.

Acknowledgments

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Table 1: Force relative error. The parameters used are $L = 8$, and $ws = 1.7$.

Particles	Force relative error	
	Original	Present
10000	$9.0 \cdot 10^{-7}$	$1.3 \cdot 10^{-6}$
20000	$4.8 \cdot 10^{-7}$	$7.6 \cdot 10^{-7}$
30000	$6.4 \cdot 10^{-7}$	$9.6 \cdot 10^{-7}$
40000	$8.6 \cdot 10^{-7}$	$1.3 \cdot 10^{-6}$
50000	$8.7 \cdot 10^{-7}$	$1.2 \cdot 10^{-6}$

Figure 1: CPU time for the computation of forces versus the number of particles in the system. The parameters used are $L = 8$, and $ws = 1.7$.

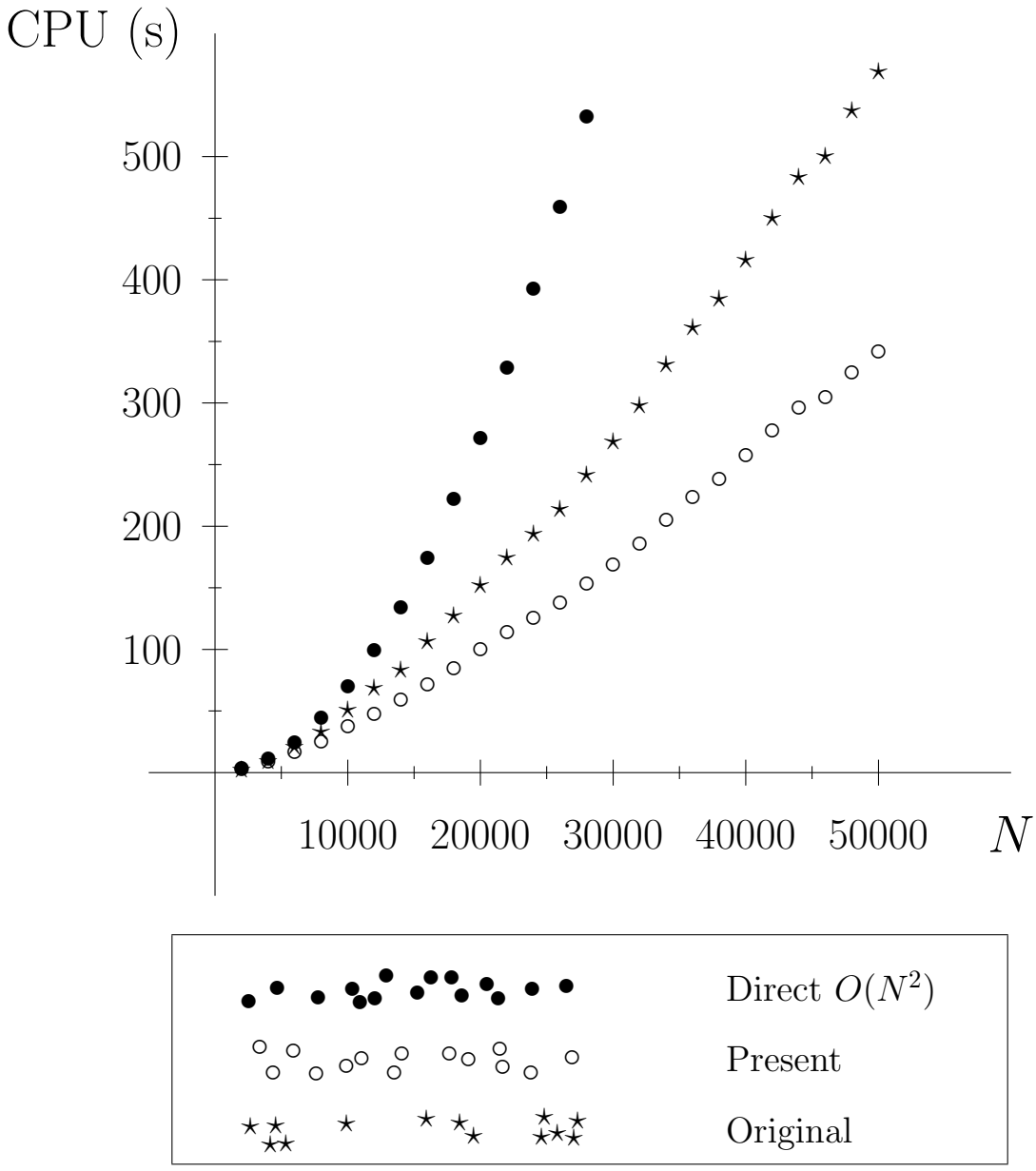

Figure 1: CPU time for the computation of forces versus the number of particles in the system. The parameters used are $L = 8$, and $ws = 1.7$.